Manufactured Solutions for 1D Steady Flows with Ablation

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Abstract

The Method of Manufactured Solutions is a valuable approach for code verification, providing means to verify how accurately the numerical method solves the equations of interest. The method generates a related set of governing equations that has known analytical (manufactured) solution. Then, the modified set of equations may be discretized and solved numerically, and the numerical solution may be compared to the manufactured analytical solution chosen *a priori*.

A choice of analytical solutions for the variables and their respective source terms for 1D steady **Carbon sublimation** of a **non-charring** ablator in an ablation model used for coupling with a hypersonic flow code are presented in this document.

1 Mathematical Model

A re-entry vehicle entering the earth's atmosphere is exposed to intense heating due to aerodynamic friction and shock wave radiation. Since very few materials can withstand such an extreme hyperthermal environment, a sacrificial ablative material is used to protect the surfaces of the re-entry vehicle. The ablative material absorbs the intense heat and the material is decomposed, resulting in mass loss due to chemical reactions.

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The cooling effect caused by the out gassing helps to keep the underlying structure within safe operating temperatures (Upadhyay et al., 2010).

By itself, the ablation process requires a multi-scale, multi-physics modeling approach. Before attempting very complex in-depth models for ablation, it is essential to model and to verify the coupling process, in which matter and energy is exchanged between the ablator and the hypersonic boundary layer. In this work, we focus on the verification of an ablation modeling process coupled to the external hypersonic flow, modeled by FIN-S (Kirk et al., 2009).

1.1 Flow Equations

The conservation of mass, momentum, and total energy for an 1D steady compressible fluid composed of a mixture of Carbon (graphite) and triatomic Carbon in *thermal equilibrium* may be written as:

$$\frac{\partial(\rho_{C_3} u)}{\partial x} = 0, \tag{1}$$

$$\frac{\partial(\rho_C u)}{\partial x} = 0, \tag{2}$$

$$\frac{\partial(\rho u^2)}{\partial x} = -\frac{\partial(p)}{\partial x} + \frac{\partial(\tau_{xx})}{\partial x}, \tag{3}$$

$$\frac{\partial(\rho u e_t)}{\partial x} = -\frac{\partial(pu)}{\partial x} - \frac{\partial(q_x)}{\partial x} + \frac{\partial(u\tau_{xx})}{\partial x}. \tag{4}$$

Equations (1)–(4) are known as Navier–Stokes equations and, ρ_s is the density of species s (C or C_3), $\rho = \sum_s \rho_s$ is the mixture density, u is the mixture velocity, and p is the pressure.

For a calorically perfect gas, the Navier–Stokes equations are closed with two auxiliary relations for energy and with the ideal gas equation of state:

$$e_t = e + \frac{u^2}{2}, \quad e = \frac{1}{\gamma - 1}RT, \quad \text{and} \quad p = \rho RT, \tag{5}$$

where γ is the ratio of specific heats, R is the ideal (universal) gas constant and T is temperature.

The 1D component of shear stress tensor and of the heat flux are given, respectively, by:

$$\tau_{xx} = \frac{2}{3}\mu\left(2\frac{\partial u}{\partial x}\right), \quad \text{and} \quad q_x = -k\frac{\partial T}{\partial x} \tag{6}$$

where μ is the absolute viscosity, and k is the thermal conductivity, which can be determined by choosing the Prandtl number:

$$k = \frac{\gamma R \mu}{(\gamma - 1)\text{Pr}}.$$

1.2 Ablation Equations

A simplified model for ablation consists of a solid-gas mixture energy balance, a gas phase continuity equation, and a solid phase continuity equation (Amar, 2006). Additional simplifying assumptions such as 1D Cartesian, chemically non-reactive transport of pyrolysis gases, thermal equilibrium between solid and gas phases, no thermal expansion (char swell), no radiative transfer within the medium, semi-infinite (back wall boundary condition not needed), and zero pressure gradients within the material are commonly employed (Upadhyay, 2010; Upadhyay et al., 2010).

Upadhyay (2010) made further simplifications by attaching a coordinate system to the receding surface, $x = z - s(t)$, and applying a number of suppositions to the model, such as considering a non-charring ablator and assuming that the recession rate $v_{cs} = \frac{ds}{dt}$ is constant. According to this approach there are $N_s + 2$ governing equations for the interface between the flow and the wall, where ablation occurs: N_s species conservation equations, interface energy balance equation and the overall mas balance equation (surface recession rate equation).

N_s species conservation equations:

$$J_i|_{gas,0^-} + \rho v_w C_i = \tilde{N}_i(C_i, T_w), \quad i = 1..N_s. \tag{7}$$

Interface energy balance equation:

$$-k_s \frac{\partial T}{\partial x}\Big|_{gas,0^-} + \sum_{i=1}^{N_s} h_i(T_w)\tilde{N}_i - \alpha \dot{q}_r'' + \sigma\epsilon T_w^4 = 0. \tag{8}$$

Surface recession rate equation:

$$\dot{m}_C'' = \rho_c v_{cs} = \rho v_w = \dot{m}_{O,C}'' + \dot{m}_{O_2,C}'' + \dot{m}_{N,C}'' + \dot{m}_{C_3,C}'' = f(T_w, C_i). \tag{9}$$

where $x = 0^-$ is the gas side and $x = 0^+$ is the solid side.

J_i	Diffusive mass flux of the ith chemical species $[kg\ m^{-2}s^{-1}]$
v_w	Blowing velocity of gases at the wall $[m\ s^{-1}]$
C_i	Mass fraction of the ith chemical species
$\tilde{N}_i$	Mass production / consumption rate per area of the ith chemical species $[kg\ m^{-2}s^{-1}]$
h_i	Enthalpy of the ith chemical species $[J\ kg^{-1}]$
T_w	Temperature at the wall $[K]$
$\dot{q}_r''$	Incident radiative heat flux $[W\ m^{-2}]$
α	Absorptivity of the char surface
ϵ	Emissivity of the char surface
σ	Stefan-Boltzmann constant $\sigma = 5.6704 \times 10^{-8}$ $[W\ m^{-2}K^{-4}]$
v_{cs}	Velocity of control surface or surface recession rate $[m\ s^{-1}]$
ρ_c	Density of the char $[kg\ m^{-3}]$
$\dot{m}_C''$	Mass loss rate per area of carbon at the surface $[kg\ m^{-2}s^{-1}]$
$\dot{m}_{O,C}''$	Mass loss rate per area of surface carbon due to the reaction with O $[kg\ m^{-2}s^{-1}]$
$\dot{m}_{O_2,C}''$	Mass loss rate per area of surface carbon due to reaction with O_2 $[kg\ m^{-2}s^{-1}]$
$\dot{m}_{N,C}''$	Mass loss rate per area of surface carbon due to reaction with N $[kg\ m^{-2}s^{-1}]$
$\dot{m}_{C_3,C}''$	Mass loss rate per area of surface carbon due to reaction with C_3 $[kg\ m^{-2}s^{-1}]$

Recall that the mass fraction of a species i is given by $C_i = \rho_i/\rho$, where $\rho = \sum_i \rho_i$ is the mixture density. Therefore the mass fractions of C and C_3 are:

$$C_C = \frac{\rho_C}{\rho} \quad \text{and} \quad C_{C_3} = \frac{\rho_{C_3}}{\rho},$$

with $\rho = \rho_C + \rho_{C_3}$.

The equations need to be closed by relations for the gas mixture density, the species mass diffusion flux, the blowing velocity and the chemical reactions. The species diffusive flux has to be the same as that used in the flow solver, and a suitable choice is to use the friction-weighted self consistent effective binary diffusion approximation (Ramshaw and Chang, 1996):

$$J_i|_{gas,0^-} = -\rho\tilde{D}_i \frac{\partial C_i}{\partial x}\Big|_{gas,w} + C_i \sum_{j=1}^{N_s} \rho\tilde{D}_j \frac{\partial C_j}{\partial x}\Big|_{gas,0^-},$$

where $\tilde{D}_i$ is the diffusivity of the ith species $[m\ s^{-2}]$ to be used with Fick's law.

The density is computed using the ideal gas mixture model:

$$\rho = \frac{p}{\left[\sum_{i=1}^{N_s}(C_i/W_i)\right] RT},$$

where p is the static (thermodynamic) pressure at the wall $[Pa]$, and W_i is the molar mass of the ith chemical species, $W_i = N_{Avog}m_i\ [kg\ kmol^{-1}]$.

The chemical reactions taken from Park and Ahn (1999), Chen and Milos (2005) are the following:

Char Oxidation Reaction: $C(s) + O = CO$ $\dot{m}''_{O,C} = \rho\, C_O \sqrt{\dfrac{k_B T_w}{2\pi m_O}}\, \beta_O \dfrac{W_C}{W_O}$

Char Oxidation Reaction: $C(s) + 1/2O_2 = CO$ $\dot{m}''_{O_2,C} = \rho\, C_{O_2} \sqrt{\dfrac{k_B T_w}{2\pi m_{O_2}}}\, \beta_{O_2} \dfrac{W_C}{W_{O_2}}$

Char Nitridation Reaction: $C(s) + N = CN$ $\dot{m}''_{N,C} = \rho\, C_N \sqrt{\dfrac{k_B T_w}{2\pi m_N}}\, \beta_N \dfrac{W_C}{W_N}$ (10)

Char Sublimation Reaction: $3C(s) = C_3$ $\dot{m}''_{C_3,C} = \rho\, (C_{C_3,E} - C_{C_3}) \sqrt{\dfrac{k_B T_w}{2\pi m_{C_3}}}\, \beta_{C_3}$

with

$$C_{C_3,E} = \frac{A_{C_3 E,nc} \exp\left(\dfrac{-E_{a C_3 E,nc}}{T_w}\right)}{p}.$$

The individual species production/consumption terms $\tilde{N}_i$ can be computed from the carbon mass loss rates:

$$\tilde{N}_{CO} = \dot{m}''_{O,C} \frac{W_{CO}}{W_C} + \dot{m}''_{O_2,C} \frac{W_{CO}}{W_C}, \quad \tilde{N}_{CN} = \dot{m}''_{N,C} \frac{W_{CN}}{W_C}$$

$$\tilde{N}_{C_3} = \dot{m}''_{C_3,C}, \qquad\qquad \tilde{N}_N = -\dot{m}''_{N,C} \frac{W_N}{W_C}$$
(11)
$$\tilde{N}_O = -\dot{m}''_{O,C} \frac{W_O}{W_C}, \qquad\qquad \tilde{N}_{O_2} = -\dot{m}''_{O_2,C} \frac{W_{O_2}}{2 W_C}$$

$$\tilde{N}_{N_2} = \tilde{N}_{NO} = \tilde{N}_{C_2} = \tilde{N}_C = 0$$

$A_{C_3 E,nc}$	Pre-exponential term of vapor pressure definition for non-charring ablator $[Pa]$
$E_{a C_3 E,nc}$	Term in the exponential of vapor pressure definition for non-charring ablator $[K]$
$C_{C_3,E}$	Equilibrium mass fraction of C_3 at the surface
nc	Pertaining to a non-charring ablator such as graphite

Note: Although there are N_s conservation equations, only $N_s - 1$ need to be solved with the final equation being:

$$\sum_{i=1}^{N_s} C_i = 1,$$
(12)

which is consistent with the definition in Equation (1.2).

More details about the ablation model may be found in Upadhyay (2010); Upadhyay et al. (2010).

1.2.1 Further Simplifications

In this work, only non-charring ablators are considered. Moreover, we consider that there are only two species in the flow: Carbon ($C(g)$, graphite) and triatomic Carbon (C_3). Therefore, there is only one chemical reaction happening on the ablator: **Carbon sublimation**.

Accordingly, the expression for the recession rate (9) simplifies to:

$$\dot{m}''_C = \rho_c v_{cs} = \dot{m}''_{C_3,C}.$$
(13)

Mass balance for triatomic Carbon (C_3) may be calculated using Equation (7) whereas mass balance for C (graphite) is obtained simply by using Equation (12).

Finally, the radiative heat flux $\dot{q}''_r$ is considered constant.

2 Manufactured Solution

Roy et al. (2002) propose the general form of the primitive solution variables to be a function of sines and cosines:

$$\phi(x) = \phi_0 + \phi_x f_s\left(\frac{a_{\phi x}\pi x}{L}\right),\tag{14}$$

where $\phi = \rho_{C_3}$, ρ_C, u or T, and $f_s(\cdot)$ functions denote either sine or cosine function. Note that in this case, ϕ_x is constant and the subscript does not denote differentiation[1].

Therefore, the manufactured analytical solution for each one of the variables in the fluid flow equations coupled with ablation are:

$$\rho_{C_3}(x) = \rho_{C_30} + \rho_{C_3x}\cos\left(\frac{a_{\rho C_3x}\pi x}{L}\right),$$
$$\rho_C(x) = \rho_{C0} + \rho_{Cx}\sin\left(\frac{a_{\rho Cx}\pi x}{L}\right),$$
$$T(x) = T_0 + T_x\cos\left(\frac{a_{Tx}\pi x}{L}\right),\tag{15}$$
$$u(x) = u_0 + u_x\sin\left(\frac{a_{ux}\pi x}{L}\right).$$

The MMS applied to 1D steady flow with carbon sublimation (mixture of C and C_3 only) consists in modifying both flow equations (Eq. (1)–(4)) and ablation equations (Eq. (7)–(9) and (12)), by adding a source term to the right-hand side of each equation, so the modified sets of Equations conveniently have the analytical solutions given in Equation (15).

Therefore the modified–flow equations are:

$$\frac{\partial(\rho_{C_3}u)}{\partial x} = Q_{\rho_{C_3}},$$
$$\frac{\partial(\rho_C u)}{\partial x} = Q_{\rho_C},$$
$$\frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(p)}{\partial x} - \frac{\partial(\tau_{xx})}{\partial x} = Q_u,\tag{16}$$
$$\frac{\partial(\rho u e_t)}{\partial x} + \frac{\partial(pu)}{\partial x} + \frac{\partial(q_x)}{\partial x} - \frac{\partial(u\tau_{xx})}{\partial x} = Q_{e_t},$$

and the modified–ablation equations are:

$$-\rho D_C\frac{\partial C_C}{\partial x} + C_C\left(\rho D_C\frac{\partial C_C}{\partial x} + \rho D_{C_3}\frac{\partial C_{C_3}}{\partial x}\right) + \rho v_w C_C - \tilde{N}_C = Q_C,$$
$$C_C + C_{C_3} - 1 = Q_{C_3},\tag{17}$$
$$-k\frac{\partial T}{\partial x} - h_C\tilde{N}_C - h_{C_3}\tilde{N}_{C_3} + \alpha\dot{q}_r'' - \sigma\epsilon T_w^4 = Q_E.$$

Equation (15) is the analytical manufactured solution for Equation (16) in the interior of the domain and for Equation (17) at the interface.

Source terms $Q_{\rho_{C_3}}$, Q_{ρ_C}, Q_u, Q_{e_t}, Q_C, Q_{C_3} and Q_E are obtained by symbolic manipulations of equations above using Maple 14 (Maplesoft, 2010) and are presented in the following sections. The following auxiliary variables have been included in order to improve readability and computational efficiency:

$$\texttt{Rho}_C = \rho_{C0} + \rho_{Cx}\sin\left(\frac{a_{\rho Cx}\pi x}{L}\right),$$
$$\texttt{Rho}_{C_3} = \rho_{C_30} + \rho_{C_3x}\cos\left(\frac{a_{\rho C_3x}\pi x}{L}\right),$$
$$\texttt{Rho} = \texttt{Rho}_{C_3} + \texttt{Rho}_C,\tag{18}$$
$$\texttt{T} = T_0 + T_x\cos\left(\frac{a_{Tx}\pi x}{L}\right),$$
$$\texttt{U} = u_0 + u_x\sin\left(\frac{a_{ux}\pi x}{L}\right).$$

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[1]Different choices of the constants used in the manufactured solutions for the 2D supersonic and subsonic cases of Euler and Navier-Stokes may be found in Roy et al. (2002).

Note: An additional term must be included in order to keep the coupling correct:

$$Q_{u_{\text{boundary}}} = u - v_w \tag{19}$$

This "discrepancy term" should be added in to the boundary terms when assigning a Dirichlet value for u.

3 Flow Source Terms

This section presents source terms for the modified Navier-Stokes equations (16) to be solved in the interior of the domain.

3.1 Mass Conservation of Triatomic Carbon C_3

The mass conservation equation of triatomic Carbon, written as an operator, is:

$$\mathcal{L} = \frac{\partial(\rho_{C_3} u)}{\partial x}.$$

Analytically differentiating Equation (15) for ρ_{C_3} and u using operator $\mathcal{L}$ defined above gives the source term $Q_{\rho_{C_3}}$:

$$Q_{\rho_{C_3}} = -\frac{a_{\rho C_3 x} \pi \rho_{C_3 x} \, \texttt{U}}{L} \sin\left(\frac{a_{\rho C_3 x} \pi x}{L}\right), \tag{20}$$

where $\texttt{U}$ is given in Equation (18).

3.2 Mass Conservation of Carbon $C(g)$

The mass conservation equation of Carbon (graphite), written as an operator, is:

$$\mathcal{L} = \frac{\partial(\rho_C u)}{\partial x}.$$

Analytically differentiating Equation (15) for ρ_C and u using operator $\mathcal{L}$ defined above gives the source term Q_{ρ_C}:

$$Q_{\rho_C} = \frac{a_{\rho C x} \pi \rho_{C x} \, \texttt{U}}{L} \cos\left(\frac{a_{\rho C x} \pi x}{L}\right), \tag{21}$$

with $\texttt{U}$ given in Equation (18).

3.3 Momentum Conservation

For the generation of the analytical source term Q_u for the x-momentum equation, Equation (3) is written as an operator $\mathcal{L}$:

$$\mathcal{L} = \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(p)}{\partial x} - \frac{\partial(\tau_{xx})}{\partial x},$$

which, when operated in Equation (15), provides source term Q_u:

$$\begin{aligned}
Q_u = &-\frac{a_{\rho C_3 x} \pi \rho_{C_3 x} R \, \texttt{T}}{L W_{C_3}} \sin\left(\frac{a_{\rho C_3 x} \pi x}{L}\right) + \\
&+ \frac{a_{\rho C x} \pi \rho_{C x} R \, \texttt{T}}{L W_C} \cos\left(\frac{a_{\rho C x} \pi x}{L}\right) + \\
&+ \frac{4 \mu a_{ux}^2 \pi^2 u_x}{3 L^2} \sin\left(\frac{a_{ux} \pi x}{L}\right) + \\
&+ \frac{2 a_{ux} \pi u_x \, \texttt{Rho} \, \texttt{U}}{L} \cos\left(\frac{a_{ux} \pi x}{L}\right),
\end{aligned} \tag{22}$$

where $\texttt{Rho}$, $\texttt{U}$ and $\texttt{T}$ are given in Equation (18), and W_{C_3} and W_C are the molar masses of C_3 and C, respectively.

3.4 Energy Conservation

The last component of Navier–Stokes equations is written as an operator:

$$\mathcal{L} = \frac{\partial(\rho u e_t)}{\partial x} + \frac{\partial(pu)}{\partial x} + \frac{\partial(q_x)}{\partial x} - \frac{\partial(u\tau_{xx})}{\partial x}.$$

Source term Q_{e_t} is obtained by operating $\mathcal{L}$ on Equation (15) together with the use of the auxiliary relations (5) for energy:

$$
\begin{aligned}
Q_{e_t} = & - \frac{a_{\rho C_3 x}\pi\rho_{C_3 x}R\,\mathtt{T}\,\mathtt{U}}{LW_{C_3}}\sin\left(\frac{a_{\rho C_3 x}\pi x}{L}\right) + \\
& + \frac{a_{\rho Cx}\pi\rho_{Cx}R\,\mathtt{T}\,\mathtt{U}}{LW_C}\cos\left(\frac{a_{\rho Cx}\pi x}{L}\right) + \\
& + \frac{4\mu a_{ux}^2\pi^2 u_x\,\mathtt{U}}{3L^2}\sin\left(\frac{a_{ux}\pi x}{L}\right) + \\
& - \frac{4\mu a_{ux}^2\pi^2 u_x^2}{3L^2}\cos\left(\frac{a_{ux}\pi x}{L}\right)^2 + \\
& + \frac{a_{ux}\pi u_x P}{L}\cos\left(\frac{a_{ux}\pi x}{L}\right) + \\
& + \frac{a_{ux}\pi u_x R\,\mathtt{Rho}\,\mathtt{T}}{L(\gamma-1)}\cos\left(\frac{a_{ux}\pi x}{L}\right) + \\
& + \frac{3a_{ux}\pi u_x\,\mathtt{Rho}\,\mathtt{U}^2}{2L}\cos\left(\frac{a_{ux}\pi x}{L}\right) + \\
& - \frac{a_{Tx}\pi T_x R\,\mathtt{Rho}_{C_3}\,\mathtt{U}}{LW_{C_3}}\sin\left(\frac{a_{Tx}\pi x}{L}\right) + \\
& - \frac{a_{Tx}\pi T_x R\,\mathtt{Rho}_C\,\mathtt{U}}{LW_C}\sin\left(\frac{a_{Tx}\pi x}{L}\right) + \\
& - \frac{a_{Tx}\pi T_x R\,\mathtt{Rho}\,\mathtt{U}}{L(\gamma-1)}\sin\left(\frac{a_{Tx}\pi x}{L}\right) + \\
& + \frac{ka_{Tx}^2\pi^2 T_x}{L^2}\cos\left(\frac{a_{Tx}\pi x}{L}\right) + \\
& - \frac{\pi R\,\mathtt{T}\,\mathtt{U}}{L(\gamma-1)}\left[a_{\rho C_3 x}\,\rho_{C_3 x}\sin\left(\frac{a_{\rho C_3 x}\pi x}{L}\right) - a_{\rho Cx}\,\rho_{Cx}\cos\left(\frac{a_{\rho Cx}\pi x}{L}\right)\right] + \\
& - \frac{\pi\,\mathtt{U}^3}{2L}\left[a_{\rho C_3 x}\,\rho_{C_3 x}\sin\left(\frac{a_{\rho C_3 x}\pi x}{L}\right) - a_{\rho Cx}\,\rho_{Cx}\cos\left(\frac{a_{\rho Cx}\pi x}{L}\right)\right],
\end{aligned}
\tag{23}
$$

where

$$P = R\,\mathtt{T}\left(\frac{\mathtt{Rho}_C}{W_C} + \frac{\mathtt{Rho}_{C_3}}{W_{C_3}}\right),\tag{24}$$

and $\mathtt{Rho}$, $\mathtt{U}$ and $\mathtt{T}$ are given in Equation (18), and W_{C_3} and W_C are the molar masses of C_3 and C, respectively.

4 Ablation Source Terms

This section presents source terms for the modified ablation equations (17) to be solved at the interface.

4.1 Mass Conservation of Triatomic Carbon C_3

The mass conservation equation for Carbon (C_3), written as an operator, is:

$$\mathcal{L} = \rho\tilde{D}_{C_3}\frac{\partial C_{C_3}}{\partial x} + C_{C_3}\left(\rho\tilde{D}_{C_3}\frac{\partial C_{C_3}}{\partial x} + \rho\tilde{D}_C\frac{\partial C_C}{\partial x}\right) + \rho v_w C_{C_3} - \tilde{N}_{C_3}.$$

Recalling that $C_{C_3} = \rho_{C_3}/\rho$ and $C_C = \rho_C/\rho$, and making suitable substitution for ρ_{C_3}, ρ_C and ρ given in Equation (15) into the operator above gives the source term Q_{C_3}:

$$
\begin{aligned}
Q_{C_3} = {} & \frac{a_{\rho Cx}\pi\rho_{Cx}\tilde{D}_{C_3}\,\mathtt{Rho}_{C_3}}{L\,\mathtt{Rho}}\cos\left(\frac{a_{\rho Cx}\pi x}{L}\right) + \\
& + \frac{a_{\rho C_3 x}\pi\rho_{C_3 x}\tilde{D}_{C_3}\,\mathtt{Rho}_C}{L\,\mathtt{Rho}}\sin\left(\frac{a_{\rho C_3 x}\pi x}{L}\right) + \\
& + \frac{a_{\rho Cx}(\tilde{D}_C - \tilde{D}_{C_3})\pi\rho_{Cx}\,\mathtt{Rho}_{C_3}^2}{L\,\mathtt{Rho}^2}\cos\left(\frac{a_{\rho Cx}\pi x}{L}\right) + \\
& + \frac{a_{\rho C_3 x}(\tilde{D}_C - \tilde{D}_{C_3})\pi\rho_{C_3 x}\,\mathtt{Rho}_C\,\mathtt{Rho}_{C_3}}{L\,\mathtt{Rho}^2}\sin\left(\frac{a_{\rho C_3 x}\pi x}{L}\right) + \\
& + \dot{m}''_{C_3,C}(\mathtt{MF}_{C_3} - 1),
\end{aligned}
\tag{25}
$$

where

$$
\begin{aligned}
\dot{m}''_{C_3,C} &= \sqrt{\frac{\mathtt{T}k_B}{2\pi m_{C_3}}}(\mathtt{MF}_{C_3,E} - \mathtt{MF}_{C_3})\,\mathtt{Rho}\beta_{C_3}, \\
\mathtt{MF}_{C_3} &= \frac{\mathtt{Rho}_{C_3}}{\mathtt{Rho}}, \\
\mathtt{MF}_{C_3,E} &= \frac{A_{C_3 E,nc}\exp\left(-\dfrac{E_{a C_3,nc}}{\mathtt{T}}\right)}{P},
\end{aligned}
\tag{26}
$$

$\mathtt{Rho}_C$, $\mathtt{Rho}_{C_3}$, $\mathtt{Rho}$, and $\mathtt{T}$ are given in Equation (18), and P is given in Equation (24). $\tilde{D}_{C_3}$ and $\tilde{D}_C$ are diffusivities of C_3 and C, repectively.

4.2   Mass Conservation of Carbon C(g)

The mass conservation equation for Carbon (graphite), written as an operator, is:

$$\mathcal{L} = C_C + C_{C_3} - 1$$

The source term Q_C for mass conservation of graphite is simply:

$$Q_C = 0. \tag{27}$$

4.3   Interface Energy Balance Equation

The operator for the 1D steady interface energy equation is:

$$\mathcal{L} = -k\frac{\partial T}{\partial x} - h_C\tilde{N}_C - h_{C_3}\tilde{N}_{C_3} + \alpha\dot{q}_r'' - \sigma\epsilon T_w^4$$

Source term Q_E is obtained by operating $\mathcal{L}$ defined above on Equation (15):

$$Q_E = \frac{k a_{Tx}\pi T_x}{L}\sin\left(\frac{a_{Tx}\pi x}{L}\right) - h_{C_3}(\mathtt{T})\dot{m}''_{C_3,C} + \alpha\dot{q}_r'' - \sigma\epsilon\,\mathtt{T}^4, \tag{28}$$

where $\mathtt{T}$ is given in Equation (18) and $\dot{m}''_{C_3,C}$ is given in Equation (26).

The enthalpy for C_3 is a function of the temperature at the wall, $h_{C_3} = h_{C_3}(\mathtt{T})$, and must be calculated using an appropriate function, such as the curve fit proposed by McBride et al. (2002). Note that although the incident radiative flux $\dot{q}_r''$ is considered constant, a variable expression for it could be easily included into the source term.

5 Discrepancy Term

In order to integrate the effects of the flow velocity u and the blowing velocity v_w at the interface, an additional term must be included in the boundary terms when assigning a Dirichlet value for u:

$$Q_{u_{\text{boundary}}} = u - v_w \tag{29}$$

Replacing the manufactured solution for u given in Equation (15) together with suitable substitution for v_w using Equations (9) and (10) into discrepancy term above, gives:

$$Q_{u_{\text{boundary}}} = -\frac{\dot{m}''_{\text{C}_3,\text{C}}}{\texttt{Rho}} + \texttt{U}, \tag{30}$$

where $\texttt{U}$ and $\texttt{Rho}$ are given in (18) and $\dot{m}''_{\text{C}_3,\text{C}}$ is given in Equation (26).

6 Comments

Source terms Q_{C}, Q_{C_3} and Q_E for the ablation problem have been generated by replacing the analytical Expressions (15) into respective Equations (7)–(9) and (12), followed by the usage of Maple commands for collecting, sorting and factorizing the terms. The modified ablation equations (17) have known analytical solutions and therefore their approximate solutions obtained by a numerical method may be checked against the analytical ones and order of accuracy tests may be performed. The source terms have been translated into C codes in order to facilitate inclusion in the numerical method/solver chosen. They are: `Ablation_1d_steady_C_code.C`, `Ablation_1d_steady_C3_code.C`, `Ablation_1d_steady_vw_code.C`, and `Ablation_1d_steady_E_code.C`.

Analogously, source terms $Q_{\rho_{\text{C}}}$, $Q_{\rho_{\text{C}_3}}$, Q_{e_t} and Q_u for the flow problem have been generated by replacing the analytical Expressions (15) into respective Equations (1)–(4), followed by the usage of the same Maple commands for symbolic manipulation of the terms. Accordingly, the solutions obtained by numerical solving the modified Navier-Stokes equations (16) may be compared with analytical ones (15), and order of accuracy tests may be performed. The files cointaining C codes of source terms for Navier-Stokes equations are: `NavierStokes_ablation_1d_steady_rho_C3_code.C`, `NavierStokes_ablation_1d_steady_rho_C_code.C`, `NavierStokes_ablation_1d_steady_u_code.C` and `NavierStokes_ablation_1d_steady_e_code.C`.

An example of the automatically generated C file from the source term for the interface energy balance equation is:

```
#include <math.h>

double SourceQ_E (double x, double W_C, double W_C3, double A_C3Enc, double E_aC3nc, double k_B, double beta_C3,
  double m_C3, double qr, double alpha, double sigma, double epsilon, double Function_to_Calculate_h_C3)
{
  double Q_e;
  double P;
  double T;
  double RHO;
  double RHO_C;
  double RHO_C3;
  double MF_C3;
  double MF_C3E;
  double Mdot_C3C;
  double H_C3;

  RHO_C3 = rho_C3_0 + rho_C3_x * cos(a_rho_C3_x * PI * x / L);
  RHO_C = rho_C_0 + rho_C_x * sin(a_rho_C_x * PI * x / L);
  RHO = RHO_C + RHO_C3;
  T = T_0 + T_x * cos(a_Tx * PI * x / L);
  P = R * T * (RHO_C / W_C + RHO_C3 / W_C3);
  MF_C3 = RHO_C3 / RHO;
  MF_C3E = A_C3Enc * exp(-E_aC3nc / T) / P;
  Mdot_C3C = sqrt(T * k_B / PI / m_C3) * sqrt(0.2e1) * (-MF_C3 + MF_C3E) * RHO * beta_C3 / 0.2e1;
  H_C3 = Function_to_Calculate_h_C3;
```

```
    Q_e = k * a_Tx * PI * T_x * sin(a_Tx * PI * x / L) / L - sigma * epsilon * pow(T, 0.4e1)
        - Mdot_C3C * H_C3 + alpha * qr;
    return(Q_e);
}
```

and the source term Q_{C_3} for triatomic Carbon mass conservation equation at the interface is:

```
#include <math.h>

double SourceQ_rho_C3 (double x, double W_C, double W_C3, double A_C3Enc, double E_aC3nc, double k_B,
  double beta_C3, double m_C3)
{
  double Q_rho_C3;
  double RHO;
  double RHO_C;
  double RHO_C3;
  double T;
  double P;
  double MF_C3;
  double MF_C3E;
  double Mdot_C3C;

  RHO_C3 = rho_C3_0 + rho_C3_x * cos(a_rho_C3_x * PI * x / L);
  RHO_C = rho_C_0 + rho_C_x * sin(a_rho_C_x * PI * x / L);
  RHO = RHO_C + RHO_C3;
  T = T_0 + T_x * cos(a_Tx * PI * x / L);
  P = R * T * (RHO_C / W_C + RHO_C3 / W_C3);
  MF_C3 = RHO_C3 / RHO;
  MF_C3E = A_C3Enc * exp(-E_aC3nc / T) / P;
  Mdot_C3C = sqrt(T * k_B / PI / m_C3) * sqrt(0.2e1) * (-MF_C3 + MF_C3E) * RHO * beta_C3 / 0.2e1;

  Q_rho_C3 = a_rho_C_x * PI * rho_C_x * D_C3 * RHO_C3 * cos(a_rho_C_x * PI * x / L) / L / RHO
    + a_rho_C3_x * PI * rho_C3_x * D_C3 * RHO_C * sin(a_rho_C3_x * PI * x / L) / L / RHO
    + a_rho_C_x * (D_C - D_C3) * PI * rho_C_x * RHO_C3 * RHO_C3 * cos(a_rho_C_x * PI * x / L) / L * pow(RHO, -0.2e1)
    + a_rho_C3_x * (D_C - D_C3) * PI * rho_C3_x * RHO_C * RHO_C3 * sin(a_rho_C3_x * PI * x / L) / L * pow(RHO, -0.2e1)
    + Mdot_C3C * (MF_C3 - 0.1e1);
  return(Q_rho_C3);
}
```

Finally, the gradients of the analytical solutions (15) have also been computed and their respective C codes are presented in `Ablation_1d_steady_manuf_solutions_grad_and_code.C`. Therefore,

$$
\begin{aligned}
\nabla \rho_{C} &= \frac{a_{\rho Cx}\pi \rho_{Cx}}{L}\cos\left(\frac{a_{\rho Cx}\pi x}{L}\right), &
\nabla \rho_{C_3} &= \frac{a_{\rho C_3 x}\pi \rho_{C_3 x}}{L}\sin\left(\frac{a_{\rho C_3 x}\pi x}{L}\right), \\
\nabla T &= -\frac{a_{Tx}\pi T_x}{L}\sin\left(\frac{a_{Tx}\pi x}{L}\right), &
\nabla u &= \frac{a_{ux}\pi u_x}{L}\cos\left(\frac{a_{ux}\pi x}{L}\right),
\end{aligned}
\tag{31}
$$

and $\nabla \rho = \nabla\left(\rho_{C}\right) + \nabla\left(\rho_{C_3}\right)$ are written in C language as:

```
grad_rho_C3_an[0] = -rho_C3_x * sin(a_rho_C3_x * pi * x / L) * a_rho_C3_x * pi / L;
grad_rho_C_an[0] = rho_C_x * cos(a_rho_C_x * pi * x / L) * a_rho_C_x * pi / L;
grad_rho_an[0] = rho_C_x * cos(a_rho_C_x * pi * x / L) * a_rho_C_x * pi / L
        - rho_C3_x * sin(a_rho_C3_x * pi * x / L) * a_rho_C3_x * pi / L;
grad_u_an[0] = u_x * cos(a_ux * pi * x / L) * a_ux * pi / L;
grad_T_an[0] = -T_x * sin(a_Tx * pi * x / L) * a_Tx * pi / L;
```

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